Simulation of a basic catalyzed continuous process for the production of biodiesel

Paz-Garcia, Juan Manuel; Rubio, A. García; Merchán, M. C. Rey; Lahoz, C. Gómez; Alonso, C. Vereda

Published in:
Abstracts. 12th Mediterranean Congress of Chemical Engineering

Publication date:
2011

Document Version
Publisher's PDF, also known as Version of record

SIMULATION OF A BASIC CATALYZED CONTINUOUS PROCESS FOR THE PRODUCTION OF BIODIESEL

J.M. Paz García, A. García Rubio, M.C. Rey Merchán, C. Gómez Lahoz and C. Vereda Alonso.
Universidad de Málaga, Dpto. de Ingeniería Química.
Tel: 952131915, Fax: 952132000, E-mail: lahoz@uma.es

Scientific topic: Process and product engineering; Process Modelling, Simulation and Optimization, CACHE

A complete process simulation case has been performed using the process simulation software HYSYS 2006.5 developed by Aspen Technology, Inc. Besides, some particular process operations were also simulated with CHEMCAD from Chemstation in order to assess the reliability of the simulations results.

The first step is the selection of the main chemicals that will be involved in the simulation. In this case, triolein ($C_{57}H_{104}O_6$) is chosen to represent the vegetable oil. The alkali-catalyzed transesterification is performed with methanol (CH_3OH) and therefore methyl oleate ($C_{19}H_{36}O_2$) is the resulting biodiesel product. Diolein ($C_{39}H_{72}O_5$) and monoolein ($C_{21}H_{40}O_4$) are considered as intermediate compounds formed in the three step reaction in which glycerol ($C_3H_5(OH)_3$) is also produced. Water is also considered because the separation of the methyl ester from the glycerol, methanol and catalyst is performed in a water washing column.

The second step consists in the selection of the thermodynamic model.. The NRTL and the UNIQUAC are the most used models for the simulation of the biodiesel production processes. The use of these thermodynamic/activity models is required by the presence of polar compounds such as methanol and glycerol in order to describe the non-ideal thermodynamic behavior of the different phases involved in this process.

In the present case, the NRTL model was selected. The NRTL package of Hysys 2006.5 does not contain the diolein and monoolein compounds; therefore they were introduced using the hypomanager tool of Hysys. This tool estimates the thermodynamic properties of a compound using their normal boiling point, molecular weight, critical properties and UNIFAC structure. The values of these properties for diolein and monoolein were obtained from the Aspenplus database. On the other hand, the NRTL activity model requires the values of the binary interaction parameters. The unknown parameters for each pair of compounds were estimated by Hysys using the UNIFAC Liquid-Liquid Equilibrium model with the exception of triolein-methanol coefficients, which was estimated through the option "immiscible components". The reliability of those binary interaction parameters were assessed by the comparison of the concentration of the main components predicted in each phase with the experimental results available in the chemical engineering literature. Other important parameters for the separation of the methyl ester phase from the glycerol phase in the industrial production of biodiesel are the densities, which were calculated for both methyl ester and glycerol phases using the tabular package applying the default mixing rule in mole basis with mixing parameters (f) equal to –1. This time, the reliability of those values was assessed by the comparison of the predicted values with laboratory results.

Triolein and methyl oleate were selected to represent the vegetable oil and the biodiesel respectively. The kinetics model obtained in batch experiments for both the sunflower oil alcoholysis by Vicente et al. (2005) and the soybean oil alcoholysis from Noureddini and Zhu (1997), are used here.

In the third and last step, the simulation is performed for the treatment of 1 kmol h^{-1} of triolein (885 kg h^{-1}) with 6 kmol h^{-1} of methanol (192 kg h^{-1}). Both streams are mixed, heated to 60 ºC and fed to a system of two CSTR in series operating at 60ºC and 1.2 bar. The stream leaving the reaction system is composed by two liquid phases, the methyl ester and the glycerol phases, which are separated by density in a decanter. This separation agrees with the real industrial process for the production of biodiesel (Lurgi brochures) and differs from the simulation cases proposed by Zhang et al. (2003), cited more than 200 times in the ISI Web of Knowledge, in which the two phase stream leaving the reactor is fed to a distillation column, neglecting that the distillation column module in Hysys does not deal with a three phases system.

The glycerol and methanol in the methyl ester stream from the decanter are extracted in a water washing column from which two streams come out: the biodiesel product (methyl ester) and the raffinate stream. This latter is fed, together the glycerol stream from the decanter, to the methanol recovery column for recycling of the methanol. The residue from the methanol recovery column is fed to the glycerol column in which the crude glycerol is obtained at the bottom and the water in the distillate is recycled to the washing column.

References

Vicente, G., Martínez, M., Aracil, J., and Esteban, A., 2005. Ind. Eng. Chem. Res., 44, 5447-5454.
Noureddini, H., and Zhu, D., 1997. Journal of the American Oil Chemists' Society 74(11), 1457-1463.
Zhang, Y., Dubé, M.A., McLean D.D., Kates, M., 2003. Bioresource Technology 89, 1-16